

3-Ethyltoluene
620-14-4 | DTXSID6050386

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 160 °C

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 9.04e-01

Nearest Neighbors from the Training Set

Image not found

3-Ethyltoluene

Measured: 161

Predicted: 160

Image not found

1-Ethyl-2-methylbenzene

Measured: 165

Predicted: 160

Image not found

4-Ethyltoluene

Measured: 162

Predicted: 160

Image not found

Propylbenzene

Measured: 159

Predicted: 160

Image not found

Cumene

Measured: 152

Predicted: 160